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Nuclear Stopping Power And Its Impact On The Determination Of Electronic Stopping Power

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Abstract. As already noted by Behar et al. in the nineties, the penetration depth of heavy ions into light targets is often much larger than predicted by Ziegler's SRIM (The Stopping and Range of Ions in Matter) program. Evidently, SRIM stopping power must be too high at low energy in these cases. This leads to the question: are there any stopping power measurements that show this directly? There are a few, indeed. We first discuss the description of nuclear stopping in SRIM, and then discuss these measurements. Naturally, the contribution of nuclear stopping is large in these cases. Assuming that SRIM nuclear stopping is correct, we find that indeed, SRIM electronic stopping is much too high at low energy.

Keywords: Energy loss of ions, stopping power, stopping force, nuclear stopping power.
PACS: 30.50.Bw

INTRODUCTION

An apparent discrepancy between stopping power and penetration depth for Au ions in SiC has been found by Zhang et al[1], see Fig. 1. For 10 MeV Au ions, the experimental range, as determined by secondary ion mass spectrometry (SIMS), is 36 % above the SRIM prediction. Hence: SRIM stopping is too high in this case.

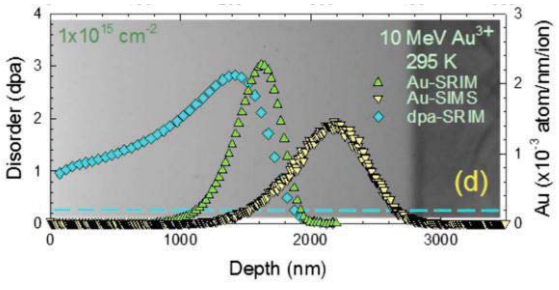

FIGURE 1. The penetration of 10 MeV Au ions into SiC, as measured by Zhang et al.[1] The experimental range (measured by means of SIMS) is 36 % above the SRIM prediction

But this problem is not new: Behar et al.[2] found already in 1995 that in most cases for heavy ions in light targets, experimental ranges exceed the SRIM[i] values by 20 – 40 %. Evidently, SRIM stopping (nuclear and/or electronic) must be too high at low energy for heavy ions.

Question: Are there any direct stopping power measurements showing that?

Answer: YES, there are!

ELECTRONIC AND "NUCLEAR" STOPPING POWER

Linear stopping power (stopping force) is defined as $S = -dE/dx$, where E is the ion energy and x is the path length. We often use the mass stopping power S/ρ, where ρ is the mass density of the material.

- Electronic stopping (collisions between ion and target electrons) leads primarily to excitation and ionization of target atoms, and to energy loss of ion.
- „Nuclear" stopping (elastic „billiard ball" collisions between ion and target atom) leads to change of direction, and to energy loss of ion. (No nuclear forces are involved!)

Fig. 2 shows the electronic and nuclear mass stopping powers for carbon and iodine ions in aluminum, calculated using SRIM[3], versus specific

[i] SRIM electronic stopping power has remained unchanged since 2003.

Application of Accelerators in Research and Industry
AIP Conf. Proc. 1525, 309-313 (2013); doi: 10.1063/1.4802339

energy, i.e., energy per nucleon. One sees that for heavier ions (higher atomic number Z_1 of the ion), the cross over point between electronic and nuclear stopping lies at higher specific energy. Hence, the greatest importance of nuclear stopping will be found for heavy ions at low energy.

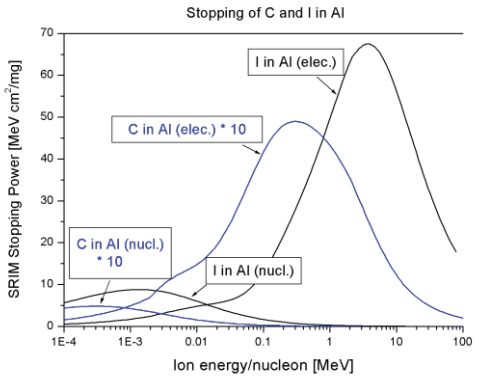

FIGURE 2. Electronic and nuclear mass stopping power for carbon and iodine ions in aluminum, calculated using SRIM.

The total stopping power is the sum of nuclear and electronic stopping power:

$$S = S_n + S_e . \tag{1}$$

The CSDA (continuous slowing down approximation) range *R* can be obtained by integrating the reciprocal of *S*:

$$R = \int_0^R dx = \int_{E_0}^{0} \frac{dE}{dE/dx} = \int_0^{E_0} \frac{dE}{-dE/dx} = \int_0^{E_0} \frac{dE}{S} \tag{2}$$

IS THE SRIM (ZBL) NUCLEAR STOPPING POWER RELIABLE?

In 1986, O'Connor and Biersack[4] wrote: "In many processes, the nuclear potential is the dominant factor in the events which lead to backscattering, sputtering, radiation and the spatial distributions of implanted ions and recoiling atoms", and this statement still holds.

This potential is normally written

$$V(r) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r} \Phi\left(\frac{r}{a}\right), \tag{3}$$

where Z_1, Z_2 are the atomic numbers of ion and atom, *e* is the electronic charge, *r* is the radius, and *a* is the „screening length". The screening function Φ is unity at $r = 0$ and decreases with increasing *r*. Using V(r), the scattering angle can be calculated in every interatomic collision.

In SRIM[3] Monte Carlo calculations, the scattering of ions is calculated using[5] the "Ziegler-Biersack-Littmark (ZBL) Universal Screening Potential"

$$\Phi_U = .1818e^{-3.2x} + .5099e^{-.9423x} + .2802e^{-.4028x} + .2817e^{-.2016x} \tag{4}$$

with the normalized radius

$$x = r / a_U , \tag{5}$$

and the screening length

$$a_U = \frac{0.8854 a_0}{Z_1^{0.23} + Z_2^{0.23}} \tag{6}$$

where a_0 is the Bohr radius. The empirical function (4) is based on calculated[5] solid-state interatomic potentials of 522 randomly chosen pairs of atoms over the range 1 - 82 for Z_1 and Z_2. It is shown[ii] in Fig. 3,

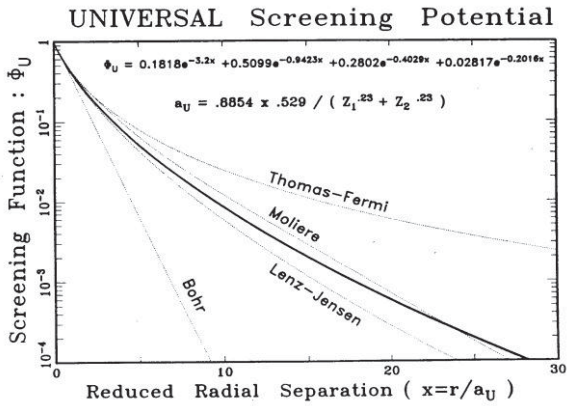

FIGURE 3. The ZBL Universal Screening Potential[5], compared to older screening models

compared to older screening models. Fig. 4 shows that the universal interatomic screening function represents the 522 calculated potentials fairly well (within 18 %), better than the older screening functions.

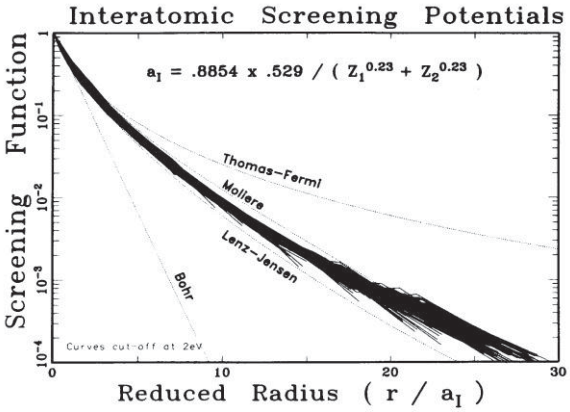

FIGURE 4. The ZBL Universal Screening Potential[5] represents the 522 calculated interatomic potentials fairly well.

[ii] Figs. 3 and 4 are taken from ref.[5], by kind permission of Jim Ziegler.

The Universal screening function Φ_U has been compared by O'Connor and Biersack[4] to over one hundred interatomic potentials derived mainly from scattering experiments[iii], and on the average, agreement has been found within 5 % between theory and experiment. The SRIM program produces values of "nuclear" stopping power by integrating the scattering over the forward hemisphere.

Until 2008, SRIM used the "Magic Formula" (eq. 4) to calculate the scattering angle. Since then, specific interatomic potentials are used[5] for the two atoms involved in the collision[iv].

EXAMPLES OF STOPPING MEASUREMENTS WITH LARGE NUCLEAR STOPPING CONTRIBUTION

There are a few measurements of stopping power in my large collection[6] of stopping data, where nuclear

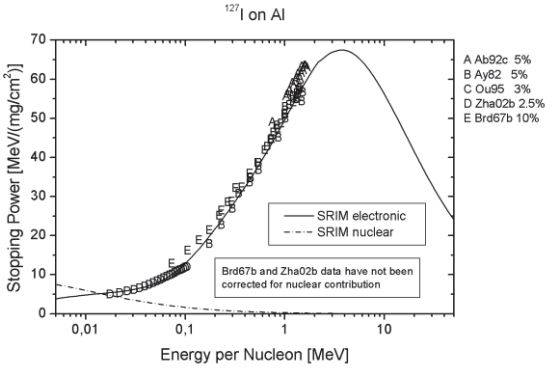

FIGURE 5. The stopping power of aluminum for iodine ions, versus specific energy. The reference codes for the experimental data can be found in ref.[6]

stopping may play an essential role. In some of these cases, the authors have not corrected for nuclear stopping. But if we want to supply this correction, we must check that scattering angles are small enough so that all scattered ions would have hit the detector.

Fig. 5 shows an example: the stopping power of aluminum for iodine ions. Subtracting the full SRIM nuclear stopping would give an experimental electronic stopping value of about zero at 0.02 MeV/nucleon, which is unreasonable. Let us assume that the transmission measurements by Zhang et al.[7, 8] designated Zha02b were carried out using an aluminum foil of 130 μg/cm^2 (4800 A) thickness, using a detector with half angle of 15°. Fig. 6 shows the result of a SRIM Monte Carlo calculation for this

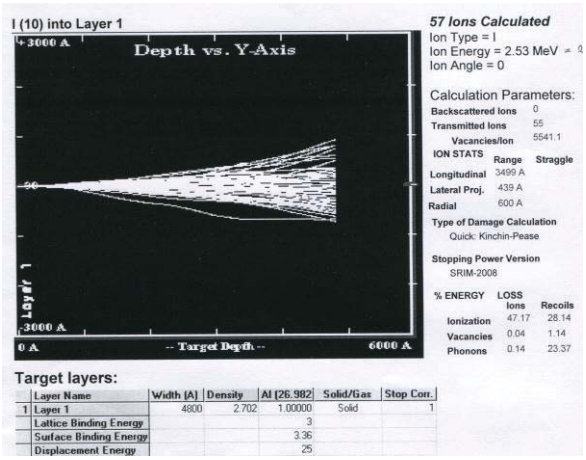

FIGURE 6. A SRIM Monte Carlo calculation for iodine ions at 0.02 MeV/nucleon, penetrating an aluminum foil of 4800 A thickness.

case. We find that only 60 % of the ions would have hit the detector. Hence, the effective SRIM nuclear contribution is smaller than what is shown in Fig. 5. Hence, SRIM electronic stopping at 0.02 MeV/nucleon is too large, as expected!

The nuclear stopping correction generally depends on geometry and on foil thickness. To provide an accurate correction for nuclear stopping, it would be extremely useful to measure the angular distribution.

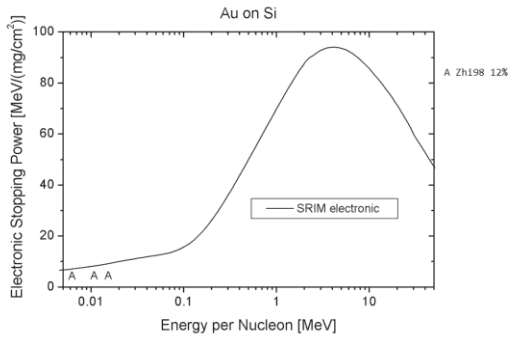

FIGURE 7. The stopping power of Au for Si ions, as measured by Yongjun Zhai et al[9].

[iii] These potential data were heavily dominated by rare gases and alkali metals. The heaviest-lightest combinations were Xe-Cl and Xe-K.

[iv] But in an Email on February 28, 2012, Jim Ziegler writes: "…In all cases of nuclear stopping, it is assumed that the ion is neutral and the target atom is in its normal crystalline state. All these assumptions make for errors, and make the nuclear stopping too large for low energies (among other problems)…
There is plenty of room for improvement, but it is a major calculation to do right since the charge state of the ion is energy dependent, and the incoming ion may take quite a while to reach equilibrium"

Fig. 7 shows the stopping of Au for Si ions. Here, the authors[9] measured ranges and found them large compared to TRIM. They deduced stopping and subtracted nuclear stopping, using Lindhard-Scharff-Schiott[10] theory. SRIM electronic stopping was again found too large.

Fig. 8 shows the stopping power of isobutane gas for U ions, measured by Barbui et al.[11] using the big

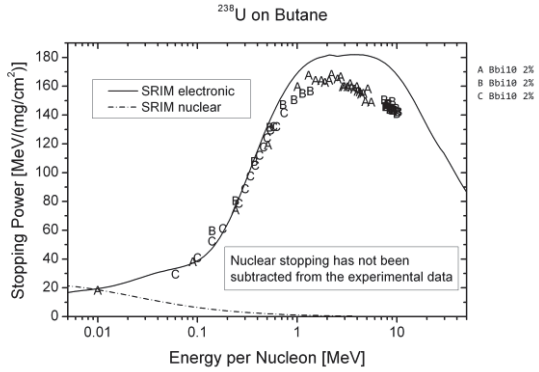

FIGURE 8. The stopping power of isobutane for U ions, as measured by Barbui et al.[11]

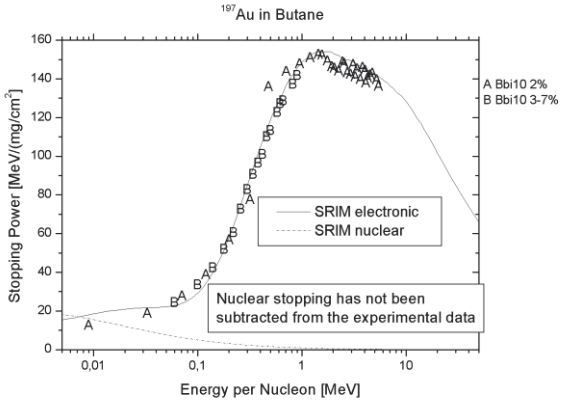

FIGURE 9. The stopping power of isobutane for Au ions, as measured by Barbui et al.[11]

superconducting solenoid at Texas A&M University. Here, the isobutane filling of the multi-anode ionization chamber detector itself was used as a target. Barbui et al. assume that the nuclear part of stopping gave no contribution, but I disagree: the heavy ion will lose most of its energy to carbon atoms via elastic collisions (nuclear stopping), and these carbon ions will spend their energy locally via electronic collisions. If some nuclear stopping is subtracted here, SRIM electronic stopping again is too large. In Fig. 9, the Barbui results for Au ions in butane again show that SRIM electronic stopping is too high at low energy, but the full nuclear stopping correction also appears too high.

At very low energies, nuclear stopping power becomes important also for light ions, as has been shown recently by Primetzhofer et al.[12]: for helium ions below 1 keV/nucleon, they find the electronic stopping power of aluminum to be smaller than determined by Martinez-Tamayo et al.[13] in 1996. But if Primetzhofer et al. add a nuclear stopping correction to their own results, they find agreement with the Martinez measurements.

CONCLUSIONS

- For stopping power measurements with heavy ions at low energy, it is imperative to correct for the nuclear contribution.
- For heavy ions at low energy, measurements of stopping show that SRIM-predicted electronic stopping power is too high: this explains why SRIM ranges are too low.
- Direct measurements of angular scattering distributions are highly desirable to check SRIM nuclear stopping.
- At very low energy, the neglect of nuclear stopping becomes significant also for stopping power measurements with light ions.

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